

# Journal of Magnetic Resonance

---

EDITOR: Wallace S. Brey, Jr.

EDITORIAL BOARD:

E. Raymond Andrew  
Edwin D. Becker  
James W. Cooper  
B. P. Dailey  
P. Diehl  
Richard Ernst  
Ray Freeman  
J. H. Goldstein  
David M. Grant

R. K. Harris  
K. H. Hausser  
Charles S. Johnson, Jr.  
J. Jonas  
Lowell Kispert  
Masaji Kubo  
George C. Levy  
Ralph Livingston

Bruce McGarvey  
Rex E. Richards  
A. Rigamonti  
Max T. Rogers  
Ian C. P. Smith  
J. B. Stothers  
Robert L. Vold  
D. E. Woessner

Volume 41, 1980



**ACADEMIC PRESS**  
**New York and London**

A Subsidiary of Harcourt Brace Jovanovich, Publishers

Copyright © 1980 by Academic Press, Inc.

All Rights Reserved

No part of this publication may be reproduced or transmitted in any form or by any means, electronic or mechanical, including photocopy, recording, or any information storage and retrieval system, without permission in writing from the copyright owner.

The appearance of the code at the bottom of the first page of an article in this journal indicates the copyright owner's consent that copies of the article may be made for personal or internal use, or for the personal or internal use of specific clients. This consent is given on the condition, however, that the copier pay the stated per copy fee through the Copyright Clearance Center, Inc. (21 Congress Street, Salem, Massachusetts 01970), for copying beyond that permitted by Sections 107 or 108 of the U.S. Copyright Law. This consent does not extend to other kinds of copying, such as copying for general distribution, for advertising or promotional purposes, for creating new collective works, or for resale. Copy fees for pre-1980 articles are the same as those shown for current articles.

MADE IN THE UNITED STATES OF AMERICA

# CONTENTS OF VOLUME 41

NUMBER 1, OCTOBER 1980

HANS DOLHAINE, MICHAEL ENGELHARDT, GERHARD HÄGELE, AND WOLFGANG KÜCKELHAUS. Application of Spectral Moments. Analysis of $^1\text{H}$ NMR Spectra of Vinylphosphonic Acid Derivatives .....	1
W. LUBITZ AND T. NYRÖNEN. $^{14}\text{N}$ and $^1\text{H}$ ENDOR and TRIPLE Resonance on Azaaromatic Radicals Produced by Sodium Reduction in Liquid Ammonia .....	17
ANDRÉ E. MERBACH, PETER MOORE, AND KENNETH E. NEWMAN. Variable-Temperature and Variable-Pressure $^1\text{H}$ NMR Studies of <i>R,S,S,R</i> -1,4,8,11-Tetramethyl-1,4,8,11-Tetraazacyclotetradecanenickel(II) Perchlorate in Aqueous Solution .....	30
G. CHIDICHIMO, F. LELJ, M. LONGERI, N. RUSSO, AND C. A. VERACINI. Complete $r^\alpha$ Structure of Selenophene Partially Oriented in a Nematic Liquid Crystal Phase by $^1\text{H}$ NMR Spectra Including $^{77}\text{Se}$ and $^{13}\text{C}$ Satellites .....	35
A. H. CLARK AND P. J. LILLFORD. Evaluation of a Deconvolution Approach to the Analysis of NMR Relaxation Decay Functions .....	42
M. CZEKALSKI, M. E. DE MILOU, AND V. J. KOWALEWSKI. A Simple Model of INDOR Spectra .....	61
HERMANN WEINGÄRTNER. The Mechanism of $^7\text{Li}$ Relaxation in a Supercooled Aqueous $\text{LiI}$ Solution .....	74
C. COUTURE, J. R. MORTON, K. F. PRESTON, AND S. J. STRACH. The EPR Spectrum of an Electron-Excess Center in $\text{Fe}(\text{CO})_2(\text{NO})_2$ Single Crystals .....	88
KIKUKO HAYAMIZU AND OSAMU YAMAMOTO. $^1\text{H}$ and $^2\text{H}$ High-Resolution NMR Spectra of Selectively Deuterated PAAs in the Nematic State ....	94
O. CLAESSEON AND A. LUND. Calculation of EPR Spectra of Triplet-State Molecules with Hyperfine and Nuclear Quadrupole Interactions ....	106
A. A. MAUDSLEY. Multiple-Line-Scanning Spin Density Imaging .....	112
J. R. MORTON AND K. F. PRESTON. Higher-Order Effects in the EPR Spectrum of $\text{F}^{33}\text{SO}_2$ .....	127
LYNN W. JELINSKI, C. E. SULLIVAN, AND D. A. TORCHIA. Effect of Proton Spin Diffusion on the $^{13}\text{C}-\{^1\text{H}\}$ NOE in Hydrated Macromolecules ....	133



RONALD G. PRATT AND JEROME L. ACKERMAN. Pulse-Pair Concept in the Design of a Microprocessor-Based Programmer for Solid-State NMR . .	140
R. B. CREEL, H. R. BROOKER, AND R. G. BARNES. Exact Analytic Expressions for NQR Parameters in Terms of the Transition Frequencies . .	146
SANDRA S. EATON, KUNDALIKA M. MORE, DANIEL L. DUBOIS, PAUL M. BOYMEL, AND GARETH R. EATON. Metal-Nitroxyl Interactions. 15. Comparison of EPR Spectra at X Band and Q Band . . . . .	150
T. T. P. CHEUNG, L. E. WORTHINGTON, P. DUBOIS MURPHY, AND B. C. GERSTEIN. Solid-State NMR Studies of Cadmium: $^{113}\text{Cd}$ - $^1\text{H}$ Cross Polarization and Magic-Angle Spinning . . . . .	158

## COMMUNICATIONS

SANKAR SENGUPTA, G. LITZISTORF, AND E. A. C. LUCKEN. The Chlorine NQR Asymmetry Parameter of Solid Molecular Chlorine	169
HIDEAKI FUJIWARA, KENSUKE TAKAHASHI, AND YOSHIO SASAKI. $^1\text{H}$ NMR Spectra of Trimethyltin Chloride Partially Oriented in a Nematic Phase . . . . .	171
B. A. CORNELL AND G. W. FRANCIS. Acyl Chain Order in Aligned Lipid Bilayers Measured by Natural-Abundance Proton-Enhanced Carbon-13 Magnetic Resonance . . . . .	175
M. M. FUSON AND J. H. PRESTEGARD. Intensity Exchange Pulses for the Extraction of Cross-Correlation Spectral Densities from Coupled $^{13}\text{C}$ Spectra of Macromolecular Systems . . . . .	179
GARETH A. MORRIS. Indirect Measurement of Proton Relaxation Rates by "INEPT" Polarization Transfer to Carbon-13: Proton Spin-Lattice Relaxation in Cholesteryl Acetate Solutions . . . . .	185
KENNETH J. FRIESEN AND RODERICK E. WASYLISHEN. Deuterium Isotope Effect on $^1J(^{15}\text{N}, ^{13}\text{C})$ in Hydrogen Cyanide . . . . .	189

## BOOK REVIEWS

MAURICE SHAMMA AND DAVID M. HINDENLANG. Carbon-13 NMR Shift Assignments of Amines and Alkaloids . . . . .	192
P. B. AYSCOUGH. Specialist Periodical Reports. Electron Spin Resonance, Vol. 5 . . . . .	192
HEINRICH NÖTH AND BERND WRACKMEYER. Nuclear Magnetic Resonance Spectroscopy of Boron Compounds. Vol. 14 of NMR, Basic Principles and Progress . . . . .	192

E. BULUGGIU AND A. VERA. Computation of Principal Values and Directions of Tensors in the Spin Hamiltonian .....	195
GEOFFREY BODENHAUSEN AND DAVID L. TURNER. Artifacts in Two-Dimensional <i>J</i> Spectra .....	200
M. PAVŠIČ AND M. SCHARA. Motional Freedom of the Acetylcholinesterase-Active-Site-Bound Spin Labels .....	207
J. D. CUTNELL, J. DALLAS, G. MATSON, G. N. LA MAR, H. RINK, AND G. RIST. Pulse Fourier Transform Water Suppression and Underwater Decoupling in Aqueous Solutions .....	213
A. LOEWENSTEIN AND A. D. GOLDSMITH. NMR Study of Nitromethane Dissolved in a Liquid Crystal .....	222
O. CLAESSON, A. LUND, J.-P. JØRGENSEN, AND E. SAGSTUEN. Electron Spin Resonance of Irradiated Crystals of 2-Thiouracil; Hyperfine Coupling Tensor for Nuclei with $I = \frac{1}{2}$ .....	229
J. P. JACOBSEN. $^{13}\text{C}$ and $^2\text{H}$ Relaxation Time Studies of Selected 1:1 Binary Mixtures: Isotope Effects on Correlation Times .....	240
J.-P. KORB AND J. MARUANI. Measurement of Spin-Spin and Spin-Lattice Relaxation Rates for Inhomogeneously Broadened Lines. II. Slow Spectral Diffusion Case .....	247
KENNETH J. PACKER AND KEVIN M. WRIGHT. <i>J</i> Order and Cross Polarization in Scalar-Coupled Spin Systems .....	268
ARTURO COLLIGIANI, CALOGERO PINZINO, MARINA BRUSTOLON, AND CARLO CORVAJA. ENDOR Determination of the $\alpha$ -Deuterium Quadrupole Tensor in the $\cdot\text{CD}(\text{COO}^-)_2$ Radical in a Single Crystal .....	279
PHILIP H. BOLTON. Enhancement of Signals from Insensitive Nuclei by Magnetization Transfer via <i>J</i> Couplings .....	287
CHARLES N. ROBINSON, CARL D. SLATER, JOHN S. COVINGTON III, CHUNG R. CHANG, LOUISE S. DEWEY, JOHN M. FRANCESCHINI, JAMES L. FRITZSCHE, JOHN E. HAMILTON, CHARLES C. IRVING, JR., JOHN M. MORRIS, DALE W. NORRIS, LARRY E. RODMAN, VERNON I. SMITH, GREGORY E. STABLEIN, AND FORREST C. WARD. Carbon-13 NMR Chemical Shift—Substituent Effect Correlations in Substituted Styrenes .....	293
K. ROTH, B. J. KIMBER, AND J. FEENEY. Data Shift Accumulation and Alternate Delay Accumulation Techniques for Overcoming the Dynamic Range Problem .....	302



STUART M. ROTHSTEIN, WILLIAM D. BELL, AND MARY FRANCES RICHARDSON. Significance Testing of Lanthanide Shift Reagent Data II .....	310
C. MAHALINGAM VENKATACHALAM AND DAN W. URRY. Analysis of Multi-site Ion Binding Using Sodium-23 NMR with Application to Channel-Forming Micellar-Packaged Malonyl Gramicidin .....	313
P. DIEHL, F. MOIA, AND H. BÖSIGER. The Use of $^{13}\text{C}$ Satellites in Spectra of Oriented Molecules: The $r_\alpha$ Structure of 1,2,4-Trichlorobenzene ....	336

#### COMMUNICATIONS

RODERICK E. WASYLISHEN, DENNIS H. MULDREW, AND KENNETH J. FRIESEN. One-Bond $^{15}\text{N}$ - $^{13}\text{C}$ Coupling Constants and $^{15}\text{N}/^{14}\text{N}$ Isotope Effects on $^{13}\text{C}$ Chemical Shielding in Some Diamagnetic Cyano Complexes .....	341
THOMAS A. EARLY, JULI FEIGON, AND DAVID R. KEARNS. Direct Measurement of Spin-Spin and Spin-Lattice Relaxation Rates of Exchangeable N-H Protons of DNA in Water .....	343
AD BAX, RAY FREEMAN, AND STEWART P. KEMPSELL. Investigation of $^{13}\text{C}$ - $^{13}\text{C}$ Long-Range Couplings in Natural-Abundance Samples .....	349
KLAUS-DIETER GRÜNINGER, ANDREAS SCHWENK, AND BRIAN E. MANN. Direct Observation of $^{103}\text{Rh}$ NMR and Relaxation Investigations by Steady-State Techniques .....	354
H. PEEMOELLER AND M. M. PINTAR. Two-Dimensional Time-Evolution Approach for Resolving a Composite Free-Induction Decay .....	358
DALLAS L. RABENSTEIN, ANVARHUSEIN A. ISAB, AND DAVID W. BROWN. Suppression of Hemoglobin Resonances in $^1\text{H}$ NMR Spectra of Intact Erythrocytes .....	361

#### NUMBER 3, DECEMBER 1980

D. W. GRANDY AND L. PETRAKIS. A High-Pressure, High-Temperature Electron Paramagnetic Resonance Cavity .....	367
ABRAHAM M. ACHLAMA. The Chemical Shift and EFG Tensors at the Carboxylic Deuterons of $\alpha$ -Oxalic Acid Dihydrate .....	374
J. HANSEN AND J. P. JACOBSEN. $^1\text{H}$ , $^2\text{H}$ , and $^{13}\text{C}$ NMR Spectra of Acetic Acid in Nematic Phases .....	381
J. TANG, L. STERNA, AND A. PINES. Anisotropic Spin-Lattice Relaxation of Deuterated Hexamethylbenzene .....	389

TED SCHAEFER AND RUDY SEBASTIAN. Comparison of LAME Analyses for an Eight-Spin System Calibrated by CW and Pulsed Methods at Different Larmor Frequencies .....	395
RICHARD K. COOPER AND JASPER A. JACKSON. Remote (Inside-Out) NMR. I. Remote Production of a Region of Homogeneous Magnetic Field ....	400
LOWELL J. BURNETT AND JASPER A. JACKSON. Remote (Inside-Out) NMR. II. Sensitivity of NMR Detection for External Samples .....	406
JASPER A. JACKSON, LOWELL J. BURNETT, AND J. FRANK HARMON. Remote (Inside-Out) NMR. III. Detection of Nuclear Magnetic Resonance in a Remotely Produced Region of Homogeneous Magnetic Field	411
L. D. BOGOMOLOVA AND E. K. HENNER. The Effects of Cluster Formation of the $\text{Fe}^{3+}$ Ions in Silicate Glasses .....	422
ULDERICO SEGRE. The Influence of the Reorientational Model on Computed ST-EPR Lineshapes .....	432
R. ECKMAN, M. ALLA, AND A. PINES. Deuterium NMR in Solids with a Cylindrical Magic Angle Sample Spinner .....	440
JAMES S. HYDE AND JOHN R. PILBROW. A Moment Method for Determining Isotropic $g$ Values from Powder EPR Spectra .....	447
A. J. ZOZULIN, H. J. JAKOBSEN, T. F. MOORE, A. R. GARBER, AND J. D. ODOM. $^{13}\text{C}$ - $\{^1\text{H}, ^{11}\text{B}\}$ Triple-Resonance Experiments. Sign Determination of $^1J(^{11}\text{B}-^{11}\text{B})$ , $J(^{13}\text{C}-^{11}\text{B})$ , and $^2J(^1\text{H}-^{11}\text{B})$ in Some Organoboron Compounds .....	458
K. V. VASAVADA, J. I. KAPLAN, AND B. D. NAGESWARA RAO. Density Matrix Theory of $\text{ABC} \rightleftharpoons \text{A'B'} + \text{C'}$ Chemical Exchange: Application to $^{31}\text{P}$ NMR Spectra of Interconverting Enzyme-Bound Reactants and Products of Phosphoryl Transfer Enzymes .....	467
JEFFREY A. REIMER AND ROBERT W. VAUGHAN. Selective Proton Observed Heteronuclear Dipolar Modulated Chemical Shift Spectra in Solids .....	483

## COMMUNICATIONS

DAVID M. DODDRELL, DAVID T. PEGG, M. ROBIN BENDALL, WILLIAM M. BROOKS, AND DANNY M. THOMAS. Enhancement of $^{14}\text{N}$ Nuclear Magnetic Resonance Signals in Ammonium Nitrate Using Proton Polarization Transfer .....	492
MICHELLE S. BROIDO AND DAVID R. KEARNS. Proton NMR Evidence for an Unusual Conformation of Poly C in Solution .....	496
AD BAX, TOON MEHLKOPF, J. SMIDT, AND RAY FREEMAN. A Simple Method for Detection of Zero-Quantum Transitions in NMR ...	502



AD BAX AND RAY FREEMAN. Investigation of $^{13}\text{C}$ - $^{13}\text{C}$ Couplings in Natural Abundance Samples: The Strong Coupling Case .....	507
LANA LEE AND BRIAN D. SYKES. The Temperature Dependence of Lanthanide-Induced $^1\text{H}$ NMR Shifts Observed for the Interaction of $\text{Yb}^{3+}$ with the Calcium-Binding Protein Parvalbumin .....	512

#### BOOK REVIEWS

MARTIN M. DORIO AND JACK H. FREED. Multiple Electron Resonance Spectroscopy .....	515
LARRY KEVAN AND ROBERT N. SCHWARTZ (Editors). Time Domain Electron Spin Resonance .....	516
LAWRENCE J. BERLINER AND JACQUES REUBEN (Editors). Biological Magnetic Resonance .....	517
J. W. EMSLEY, J. FEENEY, AND L. H. SUTCLIFFE (Editors). Progress in Nuclear Magnetic Resonance Spectroscopy .....	518

ANNOUNCEMENTS AND NEWS ITEMS .....	520
------------------------------------	-----

AUTHOR INDEX FOR VOLUME 41 .....	521
----------------------------------	-----

CUMULATIVE SUBJECT INDEX FOR VOLUMES 37-41 .....	523
--	-----